(546/281.4) or (546/290) or (546/297) or (546/298) or (546/299) or (546/300) or (546/301) or (546/302)).CCLS. 881 ((504/250) or (504/251) or (504/252) or USPAT; (504/253) or (594/254) or (504/255) or US-PGPUB; (504/256) or (504/257) or (504/258)).CCLS. (504/256) or (504/257) or (504/258)).CCLS.	002/12/13 14:49 002/12/13 14:50
(546/298) or (546/299) or (546/300) or (546/301) or (546/302)).CCLS. DERWENT (504/250) or (504/251) or (504/252) or USPAT; (504/253) or (594/254) or (504/255) or US-PGPUB; (504/256) or (504/257) or (504/258)).CCLS. DERWENT	
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(504/256) or (504/257) or (504/258)).CCLS. EPO; JPO; DERWENT	
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	002/12/13 14:50
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(546/301) or (546/302)).CCLS.) or DERWENT	
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(504/256) or (504/257) or (504/258)).CCLS.)	
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EPO; JPO;	
DERWENT WARRANT AND ASSESSED TO THE PROPERTY OF THE PROPERTY O	000/10/10 14 50
	002/12/13 14:50
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(546/298) or (546/299) or (546/300) or EPO; JPO; (546/301) or (546/302)).CCLS.) or DERWENT	
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(504/253) Of (594/254) Of (504/253) Of (504/256) or (504/257) or (504/258)).CCLS.))	
and (pyridine or pyridyl or pyridinyl)	

=> d his

(FILE 'HOME' ENTERED AT 13:13:24 ON 13 DEC 2002)

	FILE	'REGISTRY'	ENTERED	AT	13:13:38	ON	13	DEC	2002	
1		STRU	CTURE UP	LOAI	DED					

L2 0 S L1 SSS SAM

L3 STRUCTURE UPLOADED

1 S L3 SSS SAM L4

STRUCTURE UPLOADED L5

1 S L5 SSS SAM L6 54 S L5 SSS FUL L7

FILE 'CAPLUS' ENTERED AT 13:20:36 ON 13 DEC 2002

14 S L7 L8

FILE 'CAOLD' ENTERED AT 13:21:17 ON 13 DEC 2002

=> s 17

0 L7 L9

=> log y

SINCE FILE TOTAL ENTRY SESSION 0.38 206.89 COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.00 -8.67 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 13:21:29 ON 13 DEC 2002

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C:\STNEXP4\QUERIES\10087066b.str

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```
1 2 3 4 5 6
chain bonds :
   1-11 5-8 8-9 11-21
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
   1-11 11-21
exact bonds :
    5-8 8-9
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
   containing 1 :
G1:0,S
G2: [*1], [*2], [*3]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
   13:Atom 14:Atom 21:CLASS
Generic attributes :
   12:
   Saturation
                          : Unsaturated
   Number of Carbon Atoms : less than 7
   Type of Ring System
                       : Monocyclic
   13:
   Saturation
                          : Unsaturated
```

chain nodes :

ring nodes :

8 9 11 12 13 14 21

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic 14: : Unsaturated Saturation

Element Count :

Node 12: Limited

C,C1-5 N,N1

Node 13: Limited

C,C4 S,S1

0,00 N,N0

=>

Uploading 10087066a.str

L1 STRUCTURE UPLOADED

.

=> d 11

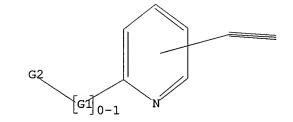
L1 HAS NO ANSWERS

L1 STI

cb 3

Hy 1

Hy 2



G1 0,S

G2 [@1],[@2],[@3]

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 17:17:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 864 TO ITERATE

100.0% PROCESSED 864 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

15517 TO 19043

PROJECTED ANSWERS: 215 TO

L2 26 SEA SSS SAM L1

=>

Uploading 10087066b.str

=>

Uploading 10087066b.str

825

26 ANSWERS

L3 STRUCTURE UPLOADED

=> d 13

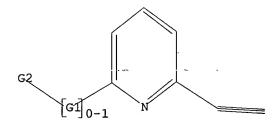
L3 HAS NO ANSWERS

L3 STR

Cb 3

Hy 1

Hy 2



G1 O,S

G2 [@1],[@2],[@3]

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

SAMPLE SEARCH INITIATED 17:20:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 160 TO ITERATE

100.0% PROCESSED 160 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

6 SEA SSS SAM L3

BATCH **COMPLETE**

PROJECTED ITERATIONS:
PROJECTED ANSWERS:

2442 TO 3958 6 TO 266

=> s 13 sss ful

L4

FULL SEARCH INITIATED 17:20:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3150 TO ITERATE

100.0% PROCESSED 3150 ITERATIONS

138 ANSWERS

SEARCH TIME: 00.00.01

L5 138 SEA SSS FUL L3

=> s 15 L6 50 L5

=> d 16 1-50 bib,ab,hitstr

```
L6
    ANSWER 1 OF 50 CAPLUS COPYRIGHT 2002 ACS
```

ΑN 2002:693101 CAPLUS

DN 137:212312

Herbicidal 2-alkynyl-pyri(mi)dines ΤI

Maier, Thomas IN

PA BASF Aktiengesellschaft, Germany

SO Eur. Pat. Appl., 28 pp. CODEN: EPXXDW

DΤ Patent

LΑ English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE -----

PΤ EP 1238586 **A**1 20020911 EP 2002-3518 20020215

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2002-59386 JP 2002322006 A2 20021108 20020305 20010309 - Pucvisional applu. PRAI US 2001-274755P MARPAT 137:212312 OS

A method of combating undesired plant growth at a locus comprises application to the locus of an effective amt. of at least one compd. I (R1 = (un)substituted alkyl, alkenyl, alkynyl, alkoxy,alkoxyalkyl, alkoxyalkoxy, haloalkyl, haloalkoxy, cyano, nitro, SF5, etc.; R3 = H, formyl, (un)substituted alkyl, alkenyl, trihydrocarbylsilyl, aryl, (un) substituted 5- or 6-membered nitrogen-contg. heteroarom. group; A = (un) substituted aryl, (un) substituted 5- or 6-membered nitrogen-contg. heteroarom. group, or (un) substituted thienyl; Z = O, S or single bond; X = N or CR2 (R2 = H, or R2 = R1); m = 0, 1, or 2) and the agronomically acceptable salts or N-oxides thereof, or herbicidal compns. contq. such compds. as active ingredients.

TT 457057-31-7 457057-33-9 457057-34-0 457057-35-1 457057-36-2 457057-37-3

457057-40-8

RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses) (herbicide)

457057-31-7 CAPLUS RN

CN Pyridine, 4-methyl-2-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-6-(phenylethynyl) - (9CI) (CA INDEX NAME)

$$_{\mathrm{F}_{3}\mathrm{C}}^{\mathrm{Me}}$$

457057-33-9 CAPLUS RN

Pyridine, 2-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-6-CN (phenylethynyl) - (9CI) (CA INDEX NAME)

RN 457057-34-0 CAPLUS

CN Pyridine, 4-methoxy-2-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-6-(phenylethynyl)- (9CI) (CA INDEX NAME)

RN 457057-35-1 CAPLUS

CN Pyridine, 4-methyl-2-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-6-[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

RN 457057-36-2 CAPLUS

CN Pyridine, 4-methyl-2-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-6-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$F_3C$$
 $C = C$
 CF_3

RN 457057-37-3 CAPLUS

CN Pyridine, 2-[(4-fluorophenyl)ethynyl]-4-methyl-6-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]- (9CI) (CA INDEX NAME)

$$F_{3}C$$
 $C = C$
 F

RN 457057-40-8 CAPLUS

CN 2-Propynal, 3-[4-methyl-6-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-2-pyridinyl]- (9CI) (CA INDEX NAME)

IT 457057-38-4 457057-39-5

RL: AGR (Agricultural use); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(herbicide)

RN 457057-38-4 CAPLUS

CN Pyridine, 2-ethynyl-4-methyl-6-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-

yl]oxy]- (9CI) (CA INDEX NAME)

RN 457057-39-5 CAPLUS

CN Pyridine, 2-(3,3-diethoxy-1-propynyl)-4-methyl-6-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & \\ N & \\ N & \\ N & \\ O & \\ N & \\ O & \\ C & \\ C & \\ C - CH-OEt \\ \end{array}$$

IT 457057-41-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. as herbicide)

RN 457057-41-9 CAPLUS

CN Pyridine, 4-methyl-2-(4-methyl-3-penten-1-ynyl)-6-[[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]- (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 2 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 2002:460725 CAPLUS
- DN 137:337556
- TI Electronic coupling in 6,6"-donor-substituted terpyridines: tuning of the mixed valence state by proton and metal ion complexation
- AU Bueschel, Michael; Helldobler, Markus; Daub, Joerg
- CS Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg, D-93040, Germany
- Chemical Communications (Cambridge, United Kingdom) (2002), (13), 1338-1339
 CODEN: CHCOFS; ISSN: 1359-7345
- PB Royal Society of Chemistry
- DT Journal
- LA English
- AB 6,6''-Terpyridyl-bishydroquinone conjugates are synthesized by Pd-catalyzed cross-coupling and their conformational switching, triggered by protons, zinc(II) or cobalt(II), is studied by cyclovoltammetry and in situ UV/Vis/NIR and FT-IR spectroelectrochem.
- IT 474265-93-5

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (FT-IR spectroelectrochem., cyclovoltammetry, and electronic spectroscopy study on electronic coupling in terpyridyl-bishydroquinone conjugates)

- RN 474265-93-5 CAPLUS
- CN INDEX NAME NOT YET ASSIGNED

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 2002:232594 CAPLUS

DN 137:94079

TI Structural characterisation of a series of acetylide-functionalised oligopyridines and the synthesis, characterisation and optical spectroscopy of platinum di-ynes and poly-ynes containing oligopyridyl linker groups in the backbone

AU Khan, Muhammad S.; Al-Mandhary, Muna R. A.; Al-Suti, Mohammed K.; Hisahm, Abdul Khader; Raithby, Paul R.; Ahrens, Birte; Mahon, Mary F.; Male, Louise; Marseglia, Elisabeth A.; Tedesco, Emilio; Friend, Richard H.; Koehler, Anna; Feeder, Neil; Teat, Simon J.

CS Department of Chemistry, College of Science, Sultan Qaboos University, Sultanate of Oman, Oman

SO Journal of the Chemical Society, Dalton Transactions (2002), (7), 1358-1368

CODEN: JCSDAA; ISSN: 1472-7773

PB Royal Society of Chemistry

DT Journal

LA English

A series of trimethylsilyl-protected bis(ethynyl)oligopyridine derivs. AB Me3SiC.tplbond.C-R-C.tplbond.C-SiMe3 (R = 2,2'-bipyridine-5,5'-diyl (1a), 2,2'-bipyridine-6,6'-diyl (2a), 2,2':6',2''-terpyridine-6,6''-diyl (3a), 4'-phenyl-2,2':6',2''-terpyridine-6,6''-diyl (4a)) has been synthesized and 2a-4a have been characterized by single crystal X-ray crystallog. corresponding terminal di-ynes H-C.tplbond.C-R-C.tplbond.CH (1b-4b) and their dinuclear platinum(ii) complexes trans-[(Et3P)2(Ph)Pt-C.tplbond.C-R-C.tplbond.C-Pt(Ph)(Et3P)2] (1M-4M) have been characterized spectroscopically and by single-crystal X-ray crystallog. for 2M. Novel platinum(ii) poly-yne polymers trans-[Pt(PBun3)2-C.tplbond.C-R-C.tplbond.C-]n (1P-4P) contq. the oligopyridyl linker groups in the backbone have been synthesized by the CuI-catalyzed dehydrohalogenation polycondensation reaction of 1b-4b and trans-[(Bu3P)2PtCl2] in Pri2NH-CH2Cl2. polymeric materials exhibit decreasing thermal stability with increasing no. of pyridine units in the linker group. In the absorption and phosphorescence spectra, the platinum(ii) poly-yne and di-yne complexes 1P, 1M show red shifts whereas the complexes 2P-3P, 2M-3M show blue shifts of the S1 and T1 states. At room temp., the phosphoresence spectra indicate some excimer formation whereas at 10 K, only intra-chain emission occurs. The results of the photophys. studies are compared with those obtained for other platinum(ii)-contg. poly-ynes and related organometallic polymers.

IT 133810-42-1P 133810-47-6P 133810-48-7P 133826-69-4P 352010-48-1P 442157-32-6P 442157-34-8P 442157-35-9P 442157-36-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(acetylide-functionalized oligopyridines and platinum di-ynes and poly-ynes contg. oligopyridyl linker)

RN 133810-42-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-diethynyl- (9CI) (CA INDEX NAME)

RN 133810-47-6 CAPLUS

CN 2,2':6',2''-Terpyridine, 4'-phenyl-6,6''-bis[(trimethylsilyl)ethynyl]-(9CI) (CA INDEX NAME)

Me₃Si-C
$$\equiv$$
C \rightarrow N \rightarrow N \rightarrow C \equiv C-SiMe₃

RN 133810-48-7 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-diethynyl-4'-phenyl- (9CI) (CA INDEX NAME)

$$HC = C$$
 N
 N
 $C = CH$

RN 133826-69-4 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

$$Me_3Si-C = C$$
 N
 N
 $C = C-SiMe_3$

RN 352010-48-1 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-diethynyl- (9CI) (CA INDEX NAME)

RN 442157-32-6 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-bis[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

RN 442157-34-8 CAPLUS

CN Platinum, [.mu.-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)]diphenyltetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)

RN 442157-35-9 CAPLUS

CN Platinum, diphenyl[.mu.-([2,2':6',2''-terpyridine]-6,6''-diyldi-2,1-ethynediyl)]tetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)

RN 442157-36-0 CAPLUS

CN Platinum, diphenyl[.mu.-[(4'-phenyl[2,2':6',2''-terpyridine]-6,6''-diyl)di-2,1-ethynediyl]]tetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)

IT 442157-40-6P 442157-42-8P 442157-44-0P 442157-46-2P 442157-47-3P 442157-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (acetylide-functionalized oligopyridines and platinum di-ynes and poly-ynes contg. oligopyridyl linker)

RN 442157-40-6 CAPLUS

CN Platinum, [6-(ethynyl-.kappa.C2)-6'-ethynyl-2,2'-bipyridinato(2-)]bis(tributylphosphine)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 442157-39-3

CMF C38 H60 N2 P2 Pt

CCI CCS

$$(n-Bu) 3P - Pt \xrightarrow{P (Bu-n) 3} C = C$$

RN 442157-42-8 CAPLUS

CN Platinum, [6-(ethynyl-.kappa.C2)-6''-ethynyl-2,2':6',2''-terpyridinato(2-)]bis(tributylphosphine)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 442157-41-7

CMF C43 H63 N3 P2 Pt

CCI CCS

RN 442157-44-0 CAPLUS

CN Platinum, [6-(ethynyl-.kappa.C2)-6''-ethynyl-4'-phenyl-2,2':6',2''-terpyridinato(2-)]bis(tributylphosphine)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 442157-43-9

CMF C49 H67 N3 P2 Pt

CCI CCS

RN 442157-46-2 CAPLUS

CN Platinum, dichlorobis(tributylphosphine)-, (SP-4-1)-, polymer with 6,6'-diethynyl-2,2'-bipyridine (9CI) (CA INDEX NAME)

CM 1

CRN 133810-42-1 CMF C14 H8 N2

CM 2

CRN 15391-01-2 CMF C24 H54 C12 P2 Pt CCI CCS

RN 442157-47-3 CAPLUS

CN Platinum, dichlorobis(tributylphosphine)-, (SP-4-1)-, polymer with 6,6''-diethynyl-2,2':6',2''-terpyridine (9CI) (CA INDEX NAME)

CM 1

CRN 352010-48-1 CMF C19 H11 N3

CM 2

CRN 15391-01-2

CMF C24 H54 C12 P2 Pt

CCI CCS

RN 442157-48-4 CAPLUS

CN Platinum, dichlorobis(tributylphosphine)-, (SP-4-1)-, polymer with 6,6''-diethynyl-4'-phenyl-2,2':6',2''-terpyridine (9CI) (CA INDEX NAME)

CM 1

CRN 133810-48-7 CMF C25 H15 N3

CM 2

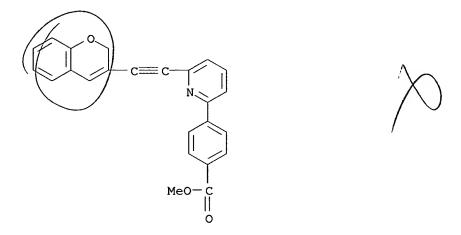
CRN 15391-01-2

CMF C24 H54 C12 P2 Pt

CCI CCS

RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 4 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 2001:867362 CAPLUS
- DN 136:151322
- TI Efficient syntheses of new heteroarotinoids through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions
- AU Alami, Mouad; Peyrat, Jean-Francois; Belachmi, Larbi; Brion, Jean-Daniel
- CS Laboratoire de Chimie Therapeutique, associe au CNRS (BioCIS), Universite Paris-Sud, Faculte de Pharmacie, Chatenay-Malabry, 92296, Fr.
- SO European Journal of Organic Chemistry (2001), (22), 4207-4212 CODEN: EJOCFK; ISSN: 1434-193X
- PB Wiley-VCH Verlag GmbH
- DT Journal
- LA English
- OS CASREACT 136:151322
- AB A convergent synthesis of heteroarotinoids bearing chromene rings in assocn. with pyridyl or ethynylpyridyl moieties, from 6-bromo-2-pyridylzinc chloride is described. This new functional heteroarylzinc reagent, readily accessible from 2,6-dibromopyridine, may undergo a selective palladium-catalyzed carbon-carbon bond-forming reaction to yield the corresponding 6-substituted-2-bromopyridines. Further manipulation of the remaining bromine atom to give the zinc deriv., and subsequent coupling with Et 4-iodobenzoate under palladium catalysis conditions afforded heteroarotinoid I. Coupling of the 6-substituted-2-bromopyridines or Me nicotinate triflate with appropriate alkynes under Sonogashira conditions give the corresponding heteroarotinoids, e.g. II.
- IT 395642-31-6P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of heteroarotinoids through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions)
- RN 395642-31-6 CAPLUS
- CN Benzoic acid, 4-[6-(2H-1-benzopyran-3-ylethynyl)-2-pyridinyl]-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 2001:518755 CAPLUS

DN 135:297298

TI A general study of the spin population of .alpha.-nitronyl nitroxide radicals: radicals with crystals presenting dominant ferro or antiferromagnetic behavior

AU Deumal, M.; Lafuente, P.; Mota, F.; Novoa, J. J.

CS Departament de Quimica Fisica and CER Quimica Teorica, Universitat de Barcelona, Barcelona, 08028, Spain

SO Synthetic Metals (2001), 122(3), 477-483 CODEN: SYMEDZ; ISSN: 0379-6779

PB Elsevier Science S.A.

DT Journal

LA English

AB The at. spin population of all the .alpha.-nitronyl nitroxide radicals whose crystals present dominant ferro or antiferromagnetic properties is computed at the B3LYP/6-31G(d) level, searching for changes and similarities in their spin distribution. The quality of the computed values is previously tested on the .alpha.-phenyl-nitronyl nitroxide radical using various basis sets. It is found that computed at. spin population presents small changes with the basis set, when the computation is done using the B3LYP d. functional. The B3LYP/6-31G(d) at. spin population of the radicals presenting dominant ferromagnetic interactions is practically independent of the system. The same is true for the antiferromägnetic systems. The two sets present also similar values. This fact is of great help when analyzing the magnetic properties of the crystals of these radicals.

IT 184240-98-0

RL: PRP (Properties)

(spin population of .alpha.-nitronyl nitroxide radicals with crystals presenting dominant ferro or antiferromagnetic behavior)

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/087,066

L6 ANSWER 6 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 2001:381068 CAPLUS

DN 135:137690

TI New Ligands Bearing Chiral Bioactive Fragments

AU Khatyr, Abderrahim; Ziessel, Raymond

CS Laboratoire de Chimie d'Electronique et de Photonique Moleculaires, CNRS ESA-7008 Ecole de Chimie Polymeres Materiaux de Strasbourg (ECPM), Strasbourg, 67087, Fr.

SO Organic Letters (2001), 3(12), 1857-1860 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 135:137690

This work presents reliable and practical synthetic routes for constructing hybrid mols. having both a chelating center and a useful biofunction. Key synthetic step is the sequential cross-coupling reaction between (ethynyl)oligopyridines and L-3-(iodo)tyrosine derivs. For example, tyrosine-oligopyridine derivs. I (R = H, COPh) are synthesized from the cross-coupling reaction of (iodo)tyrosines II (R = H, COPh) with (ethynyl)oligopyridine deriv. III in the presence of Pd(PPh3)Cl2, CuI and i-Pr2NH2 in THF.

IT 352010-48-1P 352010-49-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of (ethynyl)oligopyridine-linked tyrosines as potential bioactive chelating agents)

RN 352010-48-1 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-diethynyl- (9CI) (CA INDEX NAME)

RN 352010-49-2 CAPLUS

CN 3-Butyn-2-ol, 4,4'-[2,2':6',2''-terpyridine]-6,6''-diylbis[2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me \\ \hline \\ Me-C-C \hline \\ OH \\ \hline \\ OH \\ \hline \\ \\ N \\ \hline \\ N \\ \\ N \\ \hline \\ Me \\ \hline \\ C \hline \\ C-C-Me \\ \hline \\ OH \\ \end{array}$$

IT 352010-40-3P 352010-46-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of (ethynyl)oligopyridine-linked tyrosines as potential
 bioactive chelating agents)

RN 352010-40-3 CAPLUS

CN L-Tyrosine, 3,3'=([2,2':6',2''-terpyridine]-6,6''-diyldi-2,1-ethynediyl)bis[N-benzoyl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

RN 352010-46-9 CAPLUS
CN L-Tyrosine, 3,3'-([2,2':6',2''-terpyridine]-6,6''-diyldi-2,1ethynediyl)bis[N-benzoyl-, dimethyl ester, dibenzoate (ester) (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

O C C

PAGE 2-A

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 7 OF 50 CAPLUS COPYRIGHT 2002 ACS
L6
AN
     2001:247333 CAPLUS
DN
     134:266475
     Preparation of quinuclidine compounds and drugs containing the same as the
TI
     active ingredient of squalene synthase inhibitors
     Okada, Toshimi; Kurusu, Nobuyuki; Tanaka, Keigo; Miyazaki, Kazuki;
IN
     Shinmyo, Daisuke; Sugumi, Hiroyuki; Ikuta, Hironori; Hiyoshi, Hironobu;
     Saeki, Takao; Yanagimachi, Mamoru; Ito, Masashi
     Eisai Co., Ltd., Japan; et al.
PA
     PCT Int. Appl., 267 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
                     KIND DATE
                                           APPLICATION NO. DATE
     PATENT NO.
PΙ
     WO 2001023383
                     A1
                            20010405
                                          WO 2000-JP6665
                                                            20000927
         W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, NZ, RU, US, ZA
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     AU 2000074464
                       Α5
                                           AU 2000-74464
                                                            20000927
                            20010430
                            20020626
                                           EP 2000-962889
                                                            20000927
     EP 1217001
                      Α1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
         R:
             IE, FI, CY
                                                            20020326**
     NO 2002001528"
                     A
                            20020528***
                                           NO 2002-1528
PRAI JP 1999-273905 A
                            19990928
     JP 2000-179352
                            20000615
                      Α
                            20000927
     WO 2000-JP6665
                      W
os
     MARPAT 134:266475
     Title compds. [I; wherein R1 is hydrogen or hydroxyl; HAr is an optionally
AB
     substituted arom. heterocycle; Ar is an optionally substituted arom. ring;
     W is a CH2CH2 group which may be substituted, a CH:CH group which may be
     substituted, CC, NHCO, or the like; X is a single bond, optionally
     substituted C1-6 alkylene, Q; wherein Q is oxygen, sulfur, CO, N(R2);
     wherein R2 is C1-6 alkyl or C1-6 alkoxy, NHCO, or the like], salts
     thereof, or hydrates of both, are prepd. and are useful as excellent
     squalene synthase inhibitors. Thus, the title compd. II was prepd. and
     tested.
ΙT
     332131-63-2P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
```

(prepn. of quinuclidine compds. and drugs contg. the same as active

1-Azabicyclo[2.2.2]octan-3-ol, 3-[[3-(phenylmethyl)-6-pyrazinyl-2-

ingredient of squalene synthase inhibitors)

pyridinyl]ethynyl]- (9CI) (CA INDEX NAME)

RN

CN

332131-63-2 CAPLUS

$$CH_2-Ph$$

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 2000:801544 CAPLUS

DN 134:79889

TI Spin density in interacting nitronyl nitroxide radicals

AU Pontillon, Y.; Caneschi, A.; Gatteschi, D.; Ressouche, E.; Romero, F.; Schweizer, J.; Sessoli, R.; Ziessel, R.

CS DRFMC-SPSMS-MDN, Grenoble, 38054, Fr.

SO Understanding Chemical Reactivity (2000), 21(Electron, Spin and Momentum Densities and Chemical Reactivity), 265-274
CODEN: UCREEV; ISSN: 0924-6223

PB Kluwer Academic Publishers

DT Journal

LA English

The single crystal polarized neutron investigation of the spin d. of 2 org. nitronyl nitroxide free radicals, 2-(6-ethynyl-2-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (I) and 2-(4-methylthiophenyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (II), is reported on. These radicals with ferromagnetic interactions were compared with the 2-phenyl-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (III), in which no intermol. magnetic interaction is obsd. The results are summarized and showed that the spin d. remained on the O-N-C-N-O group. The sum of the spin populations on these atoms amts. to 0.969 .mu.B for III and only 0.877 .mu.B for I and II implying a delocalization of the spin d. of the O-N-C-N-O fragment.

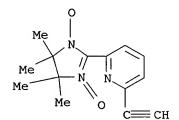
IT 184240-98-0

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(spin d. in interacting nitronyl nitroxide radicals)

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 11 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 2000:177136 CAPLUS
- DN 132:308307
- TI Synthesis of substituted pyridylpyrimidine fungicides using palladium-catalyzed cross-coupling reactions
- AU Hargreaves, Stephanie L.; Pilkington, Brian L.; Russell, Sally E.; Worthington, Paul A.
- CS Department of Chemistry, Zeneca Agrochemicals, Jealott's Hill Research Station, Bracknell, RG42 6ET, UK
- SO Tetrahedron Letters (2000), 41(10), 1653-1656 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- OS CASREACT 132:308307
- AB Various substituted Ph, pyridyl and benzyl zinc chlorides have been generated from the corresponding lithium or magnesium organometallic reagents. These have been cross-coupled with 2-(6-bromo-2-pyridyl)pyrimidines in the presence of tetrakis(triphenylphosphine)palladi um(0) to produce a series of substituted pyridylpyrimidine fungicides in 32-99% yields.
- IT 142790-12-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (pyridylpyrimidine fungicide prepn. using palladium-catalyzed cross-coupling reactions)

- RN 142790-12-3 CAPLUS
- CN Pyrimidine, 4-methyl-2-[6-(phenylethynyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 12 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 2000:83712 CAPLUS
- DN 132:230808
- TI Evidence for Transmission of Ferromagnetic Interactions through Hydrogen Bonds in Alkyne-Substituted Nitroxide Radicals: Magnetostructural Correlations and Polarized Neutron Diffraction Studies
- AU Romero, Francisco M.; Ziessel, Raymond; Bonnet, Michel; Pontillon, Yves; Ressouche, Eric; Schweizer, Jacques; Delley, Bernard; Grand, Andre; Paulsen, Carley
- CS Laboratoire de Chimie d'Electronique et de Photonique Moleculaires associe au CNRS ESA-7008, Ecole Chimie Polymeres Materiaux (ECPM), Strasbourg, 67087, Fr.
- SO Journal of the American Chemical Society (2000), 122(7), 1298-1309 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- AB A correlation between the magnetic properties and the crystal structure of the nitronyl nitroxide (NN) radical 2-(6-ethynyl-2-pyridyl)-4,4,5,5tetramethylimidazoline-1-oxyl-3-oxide (6-HC.tplbond.CPyNN, 1) and its imino nitroxide analog 2-(6-ethynyl-2-pyridyl)-4,4,5,5tetramethylimidazoline-1-oxyl (6-HC.tplbond.CPyIN, 2) was shown. susceptibility measurements on these compds. are indicative of ferromagnetic interactions between mol. units. The imino nitroxide 2 is an org. ferromagnet with crit. temp. TC = 0.19 K, whereas I behaves as an antiferromagnet ordering at the Neel temp., TN = 0.54 K. Compds. 1 and 2 are isostructural and crystallize in the P21/n space group. Their crystal packings are best described as chains of mols. linked by C.tplbond.CH.cntdot..cntdot..cntdot.O hydrogen bonds running along the [.hivin.101] direction. A comparative anal. of the structures and magnetic properties of both compds. suggests that the coupling between the mol. units along the chain is ferromagnetic. Thus, the magnetic susceptibilities of 1 and 2 were interpreted in terms of isotropic ferromagnetic Heisenberg linear chains of S = 1/2 spins. Weak values of the coupling consts. (J = +0.90 K for 1, J = +0.67 K for 2) were obtained. The spin d. distribution of radical 1 was detd. by a polarized neutron diffraction expt. to gain more insight into the mechanism of transmission of magnetic interactions. As in other NN radicals, the spin d. is concd. in the two nitroxide groups and a small neg. population is obsd. in the central carbon atom of the O-N-C-N-O fragment. However, two striking differences with respect to other nitroxides so far studied were detected. First, the spin d. is not equally shared between the two N-O functions. The oxygen atom O1, which participates in the formation of the hydrogen bond, is less populated than the free oxygen, O2. Ab initio spin d. calcns. clearly show that this effect is correlated to the presence of C.tplbond.CH.cntdot..cntdot..cntdot.O hydrogen bonds in the crystal. Second, a pos. spin d. was detected in the ethynylic hydrogen atom, H16. These two features indicate a spin d. transfer from one nitroxide group to the alkyne function of the neighboring mol.

IT 183439-03-4 184240-94-6 184240-98-0 261527-71-3

RL: PRP (Properties)

(evidence for transmission of ferromagnetic interactions through hydrogen bonds in alkyne-substituted nitroxide radicals, magnetostructural correlations and polarized neutron diffraction studies)

- RN 183439-03-4 CAPLUS
- CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-

tetramethyl- (9CI) (CA INDEX NAME)

RN 184240-94-6 CAPLUS

CN 1H-Imidazol-1-yloxy, 4,5-dihydro-4,4,5,5-tetramethyl-2-[6-[(trimethylsilyl)ethynyl]-2-pyridinyl]-, 3-oxide (9CI) (CA INDEX NAME)

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

RN 261527-71-3 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-[6-(ethynyl-d)-2-pyridinyl]-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1999:321058 CAPLUS

DN 131:73247

TI Structure - magnetism relationships in .alpha.-nitronyl nitroxide radicals

AU Deumal, Merce; Cirujeda, Joan; Veciana, Jaume; Novoa, Juan J.

CS Departament de Quimica Fisica, Facultat de Quimica Universitat de Barcelona, Barcelona, E-08028, Spain

SO Chemistry--A European Journal (1999), 5(5), 1631-1642 CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

The crystal packing of .alpha.-nitronyl nitroxide radicals with dominant AB ferromagnetic or antiferromagnetic interactions is analyzed in order to test if there are characteristic orientations of their functional groups that can be assocd. with these magnetic interactions. From a large cryst.-structure database of compds. contg. .alpha.-nitronyl nitroxide radical units (143 structures), 23 representative cases with dominant intermol. ferromagnetic interactions and 24 cases exhibiting dominant antiferromagnetic interactions were selected. The spatial distribution of the N-O.cntdot..cntdot..cntdot.O-N, C(sp3)-H.cntdot..cntdot..cntdot.ON, and C(sp2)-H.cntdot..cntdot..cntdot.ON contacts whose distance is <10 .ANG. was analyzed, with special emphasis on the 0-5-.ANG. region for the N-O.cntdot..cntdot..cntdot.O-N contacts and 0-3.8-.ANG. for the C-H-H.cntdot..cntdot..cntdot.O-N contacts. No correspondence is found between the presence of intermol. ferro- or antiferromagnetic interactions and the geometry of any of the previous isolated contacts. Therefore, there is a need to change the way in which some structure-magnetism correlations are obtained in .alpha.-nitronyl nitroxide crystals. results also show that the intermol. magnetic interaction is related to the relative orientation of the nearby mols. as a whole, i.e., with the collection of intermol. contacts made by them.

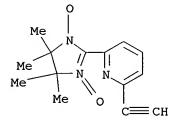
IT 184240-98-0

RL: PRP (Properties)

(structure-magnetism relationships in .alpha.-nitronyl nitroxide radicals)

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)



RE.CNT 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1999:311674 CAPLUS

DN 131:52937

TI Investigating molecular magnetism with polarized neutrons

AU Ressouche, E.

CS SPSMS-MDN, Departement de Recherche Fondamentale sur la Matiere Condensee, CEA/Grenoble, Grenoble, 38054, Fr.

SO Physica B: Condensed Matter (Amsterdam) (1999), 267-268, 27-36 CODEN: PHYBE3; ISSN: 0921-4526

PB Elsevier Science B.V.

DT Journal; General Review

LA English

AB A review with 16 refs. The detn. of magnetization d. distributions using polarized neutron diffraction has played a key role during the last 15 yr in the emerging field of mol. magnetism. In the present article, an introduction to this branch of material science and to the exptl. technique is given. The data treatment methods are briefly reviewed and some recent results are presented. A particular attention is given to the members of the nitronyl nitroxide free radicals family, which are widely used in the construction of org. magnetically ordered materials. The main features of the magnetization d. in isolated radicals are presented. Spin polarization and spin delocalization effects encountered in this class of compds. are discussed. Then the magnetic interactions with neighboring mols. can propagate through H bonds or through intermediate atoms and they modify the main features found in isolated species. In the case of a direct coordination to a transition metal ion, drastic can be the modifications on the spin d., depending on the strength of the magnetic couplings.

IT 184240-98-0

RL: PRP (Properties)

(NitPy(C.tplbond.C-H); investigating mol. magnetism with polarized neutrons in)

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 15 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1999:309462 CAPLUS
- DN 131:32109
- TI Oligosaccharide analogs of polysaccharides. Part 18. Synthesis of cyclic hybrids of 2,2'-bipyridine and acetylenosaccharides
- AU Burli, Roland; Vasella, Andrea
- CS Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.
- SO Helvetica Chimica Acta (1999), 82(4), 485-493

CODEN: HCACAV; ISSN: 0018-019X

- PB Verlag Helvetica Chimica Acta
- DT Journal
- LA English
- OS CASREACT 131:32109
- AB The efficient construction of cyclic hybrids of 2,2'-bipyridine and acetylenosaccharides from readily available building blocks is reported involving a double Castro-Stephens coupling of an O-protected and an O-unprotected, mono-C-silylated 1,4-cis-diethynylated 1,5-anhydroglucitol to 6,6'-dibromo-2,2'-bipyridine followed by oxidative cyclization of the resulting dialkynes. UV spectra of the C-alkynylated linear and cyclized bipyridines show that these ligands complex a range of metal ions.
- IT 226930-73-0P

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(cyclization and metal complexation)

- RN 226930-73-0 CAPLUS
- CN D-glycero-L-gulo-Oct-7-ynitol, 3,3'-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis[2,6-anhydro-3,7,8-trideoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

IT 226930-73-0DP, metal complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (cyclization and metal complexation)

RN 226930-73-0 CAPLUS

CN D-glycero-L-gulo-Oct-7-ynitol, 3,3'-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis[2,6-anhydro-3,7,8-trideoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

IT 226930-61-6P 226930-71-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cyclic hybrids of bipyridine and acetylenosaccharides)

RN 226930-61-6 CAPLUS

CN D-glycero-L-gulo-Oct-7-ynitol, 3,3'-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis[2,6-anhydro-3,7,8-trideoxy-4,5-bis-O-(phenylmethyl)-8-(trimethylsilyl)-, 1,1'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

RN 226930-71-8 CAPLUS

CN D-glycero-L-gulo-Oct-7-ynitol, 3,3'-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis[2,6-anhydro-3,7,8-trideoxy-8-(trimethylsilyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

Page 40

IT 226930-65-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(temp.-dependence of sp. rotation in prepn. of cyclic hybrids of bipyridine and acetylenosaccharides)

RN 226930-65-0 CAPLUS

CN D-glycero-L-gulo-Oct-7-ynitol, 3,3'-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis[2,6-anhydro-3,7,8-trideoxy-4,5-bis-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

PAGE 2-A

PAGE 2-A

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RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/087,066

L6 ANSWER 21 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1998:172272 CAPLUS

DN 128:257532

TI Reversible five-component assembly of a [2]catenane from a chiral metallomacrocycle and a dinaphtho-crown ether

AU Try, Andrew C.; Harding, Margaret M.; Hamilton, Darren G.; Sanders, Jeremy K. M.

CS School of Chemistry, University of Sydney, Sydney, 2006, Australia

SO Chemical Communications (Cambridge) (1998), (6), 723-724 CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

AB Addn. of a dinaphtho-crown ether to the components of a chiral metallomacrocycle affords a [2]catenane as the exclusive thermodn. product; the reversible assembly process is driven by a combination of zinc(II)-bipyridyl ligation and .pi.-donor/.pi.-acceptor interactions between the electronically complementary arom. components.

IT 169696-43-9

RL: RCT (Reactant); RACT (Reactant or reagent) (reversible five-component assembly of a catenane from a chiral metallomacrocycle and a dinaphtho-crown ether)

RN 169696-43-9 CAPLUS

CN Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-bis[3-(6'-methyl[2,2'-bipyridin]-6-yl)-2-propynyl]- (9CI) (CA INDEX NAME)

10/087,066

L6 ANSWER 23 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1997:450692 CAPLUS

DN 127:184601

TI Spin density in the free radical NitPy(C.tplbond.C-H)

AU Pontillon, Y.; Ressouche, E.; Romero, F.; Schweizer, J.; Ziessel, R.

CS DRFMC/SPSMS-MDN, CEA Grenoble, Grenoble, 38054, Fr.

SO Physica B: Condensed Matter (Amsterdam) (1997), 234-236, 788-789 CODEN: PHYBE3; ISSN: 0921-4526

PB Elsevier

DT Journal

LA English

AB The nitronyl nitroxide compd. NitPy(C.tplbond.C-H) (space group P21/n) crystallizes in chains with mols. connected via an H bond. Each mol. carries a delocalized, s = 1/2, unpaired electron. The intrachain magnetic interactions are pos. The authors have studied the spin d. distribution of this radical by polarized neutron diffraction. Both the spin d. population on the H, and the depletion of spin d. on the related O, give evidence that the H bond is involved in the path of the ferromagnetic interactions.

IT 184240-98-0

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(spin d. in)

RN 184240-98-0 CAPLUS

CN 1H-ImidazoI-1-ÿIoxy, 2-(6-ëthynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

L6 ANSWER 24 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1997:180899 CAPLUS

DN 126:157372

TI Construction of Preorganized Polytopic Ligands Via Palladium-Promoted Cross-Coupling Reactions

AU Grosshenny, Vincent; Romero, Francisco M.; Ziessel, Raymond

CS Laboratoire de Chimie d'Electronique et de Photonique Moleculaires, Ecole Chimie Polymeres, Strasbourg, 67008, Fr.

SO Journal of Organic Chemistry (1997), 62(5), 1491-1500 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

Rigid preorganized multitopic ligands have been designed and synthesized. AΒ The Pd(0)-catalyzed cross-coupling reaction between ethynylated derivs. of bipyridine or terpyridine and the corresponding bipyridine or terpyridine halides or triflates provide access to various homo-ditopic, hetero-ditopic, homo-tritopic, and hetero-tritopic ligands bearing acetylene or diphenylacetylene central units in fair to excellent yields. Optimal conditions were found with [Pd(PPh3)2Cl2], CuI in THF and diisopropylamine at room temp., or with [Pd(PPh3)4] in benzene and diisopropylamine at 80.degree.. When a phenylethynyl group is present in the mol., the relevant conditions involve [Pd(PPh3)4] in n-propylamine at 60.degree.. Oxidative dimerization of the ethynylated derivs. in the presence of cupric salts and oxygen gives the corresponding homo-ditopic ligands bearing diacetylene or diphenyldiacetylene as a spacer in good These methods provide a practical approach to the rational design of multichelating ligands for coordination of redox and photoactive transition metals.

IT 133810-37-4, 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl-

133810-42-1, 2,2'-Bipyridine, 6,6'-diethynyl-

RL: RCT (Reactant); RACT (Reactant or reagent)

(preorganized polytopic ligands via palladium-promoted cross-coupling reactions)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)

RN 133810-42-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-diethynyl- (9CI) (CA INDEX NAME)

IT 146548-28-9P 146548-29-0P 162318-29-8P 162318-30-1P 162318-31-2P 162318-32-3P 187026-96-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preorganized polytopic ligands via palladium-promoted cross-coupling reactions)

RN 146548-28-9 CAPLUS

CN 2,2'-Bipyridine, 6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl- (9CI) (CA INDEX NAME)

RN 146548-29-0 CAPLUS

CN 2,2'-Bipyridine, 6,6''-(1,3-butadiyne-1,4-diyl)bis[5,5'-dimethyl- (9CI) (CA INDEX NAME)

$$C = C - C = C$$

Me

Me

Me

Me

Me

RN 162318-29-8 CAPLUS

CN 2,2'-Bipyridine, 5,5'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]- (9CI) (CA INDEX NAME)

RN 162318-30-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]-(9CI) (CA INDEX NAME)

$$\underset{\mathsf{Me}}{\overset{\mathsf{N}}{\longrightarrow}} \overset{\mathsf{N}}{\overset{\mathsf{N}}{\longrightarrow}} \overset{\mathsf{C}}{=} \overset{\mathsf{C}}{\overset{\mathsf{N}}{\longrightarrow}} \overset{\mathsf{N}}{\overset{\mathsf{N}}{\longrightarrow}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}{\longrightarrow}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}}} \overset{\mathsf{N}}{\overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf{N}} \overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf{N}} \overset{\mathsf{N}}} \overset{\mathsf{N}} \overset{\mathsf$$

RN 162318-31-2 CAPLUS

CN 2,2'-Bipyridine, 4,4'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]- (9CI) (CA INDEX NAME)

$$C = C$$
 Me
 Me
 Me
 Me

RN 162318-32-3 CAPLUS

CN 2,2':6',2''-Terpyridine, 4',4''''-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis- (9CI) (CA INDEX NAME)

RN 187026-96-6 CAPLUS

CN 2,2':6',2''-Terpyridine, 4'-(4-methylphenyl)-6,6''-bis([2,2':6',2''-terpyridin]-4'-ylethynyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

$$C = C$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$C = C$$

$$N$$

$$N$$

$$C = C$$

PAGE 2-A

L6 ANSWER 25 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1996:710656 CAPLUS

DN 126:41862

TI Rapid Phosphodiester Hydrolysis by an Ammonium-Functionalized Copper(II) Complex. A Model for the Cooperativity of Metal Ions and NH-Acidic Groups in Phosphoryl Transfer Enzymes

AU Koevari, Endre; Kraemer, Roland

CS Anorganisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany

SO Journal of the American Chemical Society (1996), 118(50), 12704-12709 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

The Cu(II) complexes [(Ln)Cu(NO3)4.cntdot.2(H2O)] (n = 1: 1, n = 2: 2) of the ammonium-functionalized ligands [6,6'-(Me2HNCH2C.tplbond.C)2bpy]2+ (L1) and [6,6'-(Me3NCH2C.tplbond.C)2bpy]2+ (L2) were prepd. Hydrolysis of the activated phosphodiester bis(p-nitrophenyl) phosphate (BNPP) by these complexes in EtOH-H2O (19:1) at 20.degree. was studied. The rate consts. for cleavage of the bound phosphodiester at pH 6.6 are kcat = 4.4(.+-.0.4).times. 10-3 s-1 for (L1)Cu and kcat = 4(.+-.1) .times. 10-6 s-1 for (L1) Cu accelerates hydrolysis of BNPP 4 .times. 107-fold and is 1000 times more reactive than (L2)Cu. Probably the high reactivity of (L1)Cu is related to the interaction of the acidic -NMe2H+ group with the phosphodiester substrate. Bifunctional binding of a phosphate ester by metal coordination and H bonding with one NH4+ group is obsd. in the crystallog. characterized complex [(L1)2Cu2(1,3-.mu.-O3POPh)2(OH2)2](NO3)4.2EtOH.2H2O (3). A plausible mechanism of BNPP cleavage by (L1)Cu includes metal-hydroxide attack to the phosphodiester which is doubly activated by coordinative and H bonding. The Cu(II) complex of L1 represents a simple model for the efficient cooperativity of metal ions and NH-acidic amino acid side chains (Lys-NH4+, Arg-guanidinium, His-imidazolium) in enzymes that catalyze the cleavage of phosphate di- and monoesters.

IT 159644-79-8, 6,6'-Bis(3-dimethylaminopropynyl)-2,2'-bipyridine 159644-80-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of copper bis(dimethylammoniopropynyl)bipyridine nitrate complex)

RN 159644-79-8 CAPLUS

CN 2-Propyn-1-amine, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N-dimethyl- (9CI) (CA INDEX NAME)

$$Me_2N-CH_2-C = C$$
 N
 N
 $C = C-CH_2-NMe_2$

RN 159644-80-1 CAPLUS

CN 2-Propyn-1-amine, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N-dimethyl-, dinitrate (9CI) (CA INDEX NAME)

CM 1

CRN 159644-79-8 CMF C20 H22 N4

$$\texttt{Me}_2 \texttt{N} - \texttt{CH}_2 - \texttt{C} = \texttt{C} - \texttt{N} \\ \texttt{N} \\ \texttt{C} = \texttt{C} - \texttt{CH}_2 - \texttt{N} \\ \texttt{Me}_2 \\ \texttt{N} \\ \texttt{N} \\ \texttt{C} = \texttt{C} + \texttt{C} \\ \texttt{N} \\ \texttt{N}$$

CM 2

CRN 7697-37-2 CMF H N O3

IT 184783-26-4P, 6,6'-Bis(3-trimethylammoniopropynyl)-2,2'-bipyridine dinitrate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepr. of copper bis (dimethylammoniopropynyl) bipyridine nitrate complex)

RN 184783-26-4 CAPLUS

CN 2-Propyn-1-aminium, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N,N-trimethyl-, dinitrate (9CI) (CA INDEX NAME)

CM 1

CRN 184783-25-3 CMF C22 H28 N4

$$Me_3+N-CH_2-C \equiv C \qquad C \equiv C-CH_2-N+Me_3$$

CM 2

CRN 14797-55-8 CMF N O3

L6 ANSWER 26 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1996:660563 CAPLUS

DN 126:18551

- TI Synthesis, crystal structure and magnetic properties of novel stable nitronyl-nitroxide pyridine-based radicals (NIT)Py(X)X for Br, C .tplbond. CSiMe3, C .tplbond. CH
- AU Romero, Francisco M.; Ziessel, Raymond
- CS Laboratoire chimie, Universite Louis-Pasteur (ULP), Strasbourg, 67008, Fr.
- SO New Journal of Chemistry (1996), 20(9), 919-924 CODEN: NJCHE5; ISSN: 1144-0546
- PB Gauthier-Villars
- DT Journal
- LA English
- OS CASREACT 126:18551
- AB The synthesis of hybrid nitronyl-nitroxide pyridine-based radicals has been achieved by the use of an original protocol based on a Pd(O) cross-coupling reaction between the (NIT)Py(Br) radical and Me3SiC .tplbond. CH. The (NIT)Py(C .tplbond. CH) radical 3, obtained from the radical (NIT)Py(C .tplbond. CSiMe3) 2, forms infinite zigzag chains of mols. linked by hydrogen bonds. The magnetic susceptibility measurements show that radicals 1 and 2 are coupled antiferromagnetically while the magnetic behavior of 3 was best analyzed in terms of a one-dimensional Heisenberg chain model for ferromagnetically coupled linear arrays of spins 1/2. The best-fit data are obtained by considering an intrachain ferromagnetic interaction of J = + 1.40 K and a weak interchain antiferromagnetic interaction of zj' = -0.27 K.
- IT 184240-98-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystallog.; prepn., crystal structure and magnetic properties of stable nitronyl-nitroxide pyridine-based radicals (NIT)Py(X) (X = Br, C.tplbond.CSiMe3, C.tplbond.CH))

RN 184240-98-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

IT 184240-94-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn., crystal structure and magnetic properties of stable nitronyl-nitroxide pyridine-based radicals (NIT)Py(X) (X = Br, C.tplbond.CSiMe3, C.tplbond.CH))

RN 184240-94-6 CAPLUS

CN 1H-Imidazol-1-yloxy, 4,5-dihydro-4,4,5,5-tetramethyl-2-[6-[(trimethylsilyl)ethynyl]-2-pyridinyl]-, 3-oxide (9CI) (CA INDEX NAME)

10/087,066

- L6 ANSWER 27 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1996:656029 CAPLUS
- DN 125:328610
- TI Ferromagnetic order in a novel imino nitroxide (IT) Py(C.tplbond.CH) radical derived from 2-ethynylpyridine
- AU Romero, Francisco M.; Ziessel, Raymond; Drillon, Marc; Tholence, Jean Louis; Paulsen, Carley; Kyritsakas, Nathalie; Fisher, Jean
- CS Laboratoire Chimie Electronique Photoniques Moleculaires, Ecole Chimie Polymeres Materiaux, Strasbourg, F-67008, Fr.
- SO Advanced Materials (Weinheim, Germany) (1996), 8(10), 826-829 CODEN: ADVMEW; ISSN: 0935-9648
- PB VCH
- DT Journal
- LA English
- AB Preliminary results on the synthesis, crystal structure, and magnetic properties of the nitroxide radical I, prepd. in 6 steps starting from 6-bromopyridine-2-carbaldehyde via 6-ethynylpyridine-2-carbaldehyde, are reported.
- IT 183439-03-4P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn., crystal structure, and ferromagnetic properties of ethynylpyridine-derived imino nitroxide radical)
- RN 183439-03-4 CAPLUS
- CN 1H-Imidazol-1-yloxy, 2-(6-ethynyl-2-pyridinyl)-4,5-dihydro-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

- L6 ANSWER 28 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1996:616292 CAPLUS
- DN 125:342509
- TI Electron Delocalization in Ruthenium(II) and Osmium(II) 2,2'-Bipyridyl Complexes Formed from Ethynyl-Bridged Ditopic Ligands
- AU Grosshenny, Vincent; Harriman, Anthony; Romero, Francisco M.; Ziessel, Raymond
- CS Laboratoire de Chimie, Ecole Europeenne de Chimie, Strasbourg, F-67008, Fr.
- SO Journal of Physical Chemistry (1996), 100(44), 17472-17484 CODEN: JPCHAX; ISSN: 0022-3654
- PB American Chemical Society
- DT Journal
- LA English
- AΒ Photophys. and electrochem. properties have been recorded for a series of mono- and binuclear ruthenium(II) and osmium(II) 2,2'-bipyridyl complexes that contain an ethynyl-bridged ditopic ligand. In particular, the electrochem. properties are indicative of electron delocalization over an extended .pi. *-orbital in the .pi.-radical anions. The site of attachment of the ethynyl substituent to the 2,2'-bipyridyl ring affects the various properties, esp. absorption and emission spectral maxima. In most cases, the rates of nonradiative deactivation of the lowest-energy triplet excited states are slower than expected for a corresponding complex not possessing a conjugated substituent. This effect is rationalized in terms of electron delocalization over part of the ditopic ligand within the triplet state and its significance depends markedly on the triplet energy of the complex in question. The lowest-energy triplet mixes to some extent with an upper-lying triplet that is more strongly coupled to the ground state. According to the nature of the metal complex, this higher-energy triplet might originate from (i) charge transfer from metal center to parent ligand, (ii) a .pi.,.pi.* state localized on the ditopic ligand, or (iii) a metal-centered excited state. For the OsII complexes at 77 K electron delocalization over an extended .pi.*-orbital is accompanied by a redn. in the amt. of nuclear displacement between triplet and ground states and by a smaller vibronic coupling matrix element relative to the parent complex. These two factors combine, within the framework of the energy-gap law, to decrease the rate at which electronic energy can be dissipated among medium-frequency vibrational (i.e., -C:Cand -C:N-) modes. This realization permits a quant. explanation of the measured rate consts. for nonradiative decay of the triplet excited states of these ethynyl-substituted metal complexes.

IT 148353-62-2P 183497-78-1P

RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); PROC (Process) (photophys. and electrochem. properties of mono- and binuclear ruthenium(II) and osmium(II) bipyridyl complexes contg. ethynyl-bridged ditopic ligand)

RN 148353-62-2 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-N,N')[6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl-2,2'-bipyridine]-N,N']-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 148353-61-1 CMF C46 H38 N8 Ru CCI CCS

CM 2

CRN 16919-18-9 CMF F6 P

CCI CCS

RN 183497-78-1 CAPLUS

CN Osmium(2+), bis(2,2'-bipyridine-N,N')[6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl-2,2'-bipyridine]-N,N']-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 183497-77-0 CMF C46 H38 N8 Os

CCI CCS

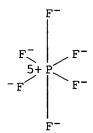
PAGE 1-A

PAGE 2-A

| Me

CM 2

CRN 16919-18-9 CMF F6 P CCI CCS



L6 ANSWER 30 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1996:182531 CAPLUS

DN 124:343062

TI Stepwise construction of polyalkyne modules grafted on oligopyridine synthons

AU Ziessel, Raymond; Suffert, Jean

CS Laboratoire Chimie, Ecole Europeenne des Hautes Etudes des Industries Chimiques de Strasbourg, Strasbourg, 67008, Fr.

SO Tetrahedron Letters (1996), 37(12), 2011-14 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

AB The stepwise homologation of the ethynylpyridines, ethynyl-2,2'-bipyridines, and ethynyol-2,2':6',6''-terpyridines with bromoethynyl(triethyl)silane using the Chodkiewicz method was reported. Chelating ligands bearing one or two triethylsilylbutadiyne, one or two triethylsilylhexatriyne subunits were synthesized and fully characterized.

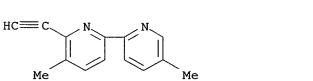
IT 133810-37-4 133810-42-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of (polyalkynyl)oligopyridines via Chodkiewicz alkynylation)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)







RN 133810-42-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-diethynyl- (9CI) (CA INDEX NAME)



IT 176715-54-1P 176715-55-2P 176715-59-6P 176715-60-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of (polyalkynyl)oligopyridines via Chodkiewicz alkynylation)

RN 176715-54-1 CAPLUS

CN 2,2'-Bipyridine, 5,5'-dimethyl-6-[4-(triethylsilyl)-1,3-butadiynyl]- (9CI) (CA INDEX NAME)



RN 176715-55-2 CAPLUS

CN 2,2'-Bipyridine, 6-(1,3-butadiynyl)-5,5'-dimethyl- (9CI) (CA INDEX NAME)

HC = C - C = C Me N N Me

RN 176715-59-6 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[4-(triethylsilyl)-1,3-butadiynyl]- (9CI) (CA INDEX NAME)

 $Et_3Si-C = C-C = C$ $C = C-SiEt_3$

RN 176715-60-9 CAPLUS

CN 2,2'-Bipyridine, 6,6'-di-1,3-butadiynyl- (9CI) (CA INDEX NAME)

 $HC \equiv C - C \equiv C$ $C = C - C \equiv CH$

IT 176715-56-3P 176715-61-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of (polyalkynyl)oligopyridines via Chodkiewicz alkynylation)

RN 176715-56-3 CAPLUS

CN 2-,2'-Bipyridine, 5,5'-dimethyl-6-[6-(triethylsilyl)-1,3,5-hexatriynyl]- (9CI) (CA INDEX NAME)

 $Et_3Si-C = C-C = C$ Me N N Me

RN 176715-61-0 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[6-(triethylsilyl)-1,3,5-hexatriynyl]- (9CI) (CA INDEX NAME)

$$Et_3Si-C = C-C = C-C = C-C = C-SiEt_3$$

L6 ANSWER 32 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1995:768726 CAPLUS

DN 123:304986

TI Guest-induced assembly of a chiral [2 + 2] metallomacrocycle

AU Bilyk, Alexander; Harding, Margaret M.

CS Sch. Chem., Univ. Sydney, 2006, Australia

SO Journal of the Chemical Society, Chemical Communications (1995), (16), 1697-8

CODEN: JCCCAT; ISSN: 0022-4936

PB Royal Society of Chemistry

DT Journal

LA English

AB A chiral metallomacrocycle, assembled from two Zn(II) ions and I, and stabilized by inclusion of o-dimethoxybenzene in the cavity, was characterized by NMR spectroscopy.

IT 169696-44-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepn. of bipyridinyl deriv. of naphthalenetetracarboxylic anhydride)

RN 169696-44-0 CAPLUS

CN 2-Propyn-1-amine, 3-(6'-methyl[2,2'-bipyridin]-6-yl)- (9CI) (CA INDEX NAME)

$$H_2N-CH_2-C \equiv C$$
 Me

IT 169696-43-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and complexation with zinc)

RN 169696-43-9 CAPLUS

CN Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-bis[3-(6'-methyl[2,2'-bipyridin]-6-yl)-2-propynyl]- (9CI) (CA INDEX NAME)

$$C = C - CH_2 - N$$

$$N - CH_2 - C = C$$

$$N$$

$$N$$

$$N$$

$$Me$$

IT 169696-43-9DP, zinc complex, methoxybenzene and nitrobenzene

inclusion compds.

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and stability consts. of)

RN 169696-43-9 CAPLUS

CN Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-bis[3-(6'-methyl[2,2'-bipyridin]-6-yl)-2-propynyl]- (9CI) (CA INDEX NAME)

$$C = C - CH_2 - N$$

$$N$$

$$N$$

$$N$$

$$Me$$

10/087,066

L6 ANSWER 34 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1995:272296 CAPLUS

DN 122:239499

TI Preparation of novel mixed tritopic oligopyridine ligands built with chelating spacers and using palladium(0) catalyzed coupling reactions

AU Romero, Francisco M.; Ziessel, Raymond

CS Laboratoire de Chimie, Institut de Physique et Chimie des Materiaux de Strasbourg, Strasbourg, 67008, Fr.

SO Tetrahedron Letters (1994), 35(49), 9203-6 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

OS CASREACT 122:239499

AB The synthesis and characterization of tritopic ligands, e.g. I, obtained by connecting two terpyridines or two bipyridines with a bis-substituted-ethynyl-bipyridine or bis-substituted-ethynyl-phenanthroline spacer are described. Palladium(0) catalyzes the coupling of the bis-ethynyl substituted central spacer with a bromo or a triflate functionalized bipyridine or terpyridine subunit. A novel trinuclear ruthenium(II) complex is also described.

IT 162318-29-8P 162318-30-1P 162318-31-2P 162318-32-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 162318-29-8 CAPLUS

CN 2,2'-Bipyridine, 5,5'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]-(9CI) (CA INDEX NAME)

RN 162318-30-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]-(9CI) (CA INDEX NAME)

RN 162318-31-2 CAPLUS

CN 2,2'-Bipyridine, 4,4'-bis[(5,5'-dimethyl[2,2'-bipyridin]-6-yl)ethynyl]- (9CI) (CA INDEX NAME)

RN 162318-32-3 CAPLUS

CN 2,2':6',2''-Terpyridine, 4',4''''-([2,2'-bipyridine]-6,6'-diyldi-2,1-ethynediyl)bis- (9CI) (CA INDEX NAME)

IT 133810-37-4 133810-42-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of novel mixed tritopic oligopyridine ligands built with
chelating spacers and using palladium catalyzed coupling reactions)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)

RN 133810-42-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-diethynyl- (9CI) (CA INDEX NAME)

Page 88

10/087,066

L6 ANSWER 35 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1995:203303 CAPLUS

DN 122:121721

TI Metal complexes of 6,6'-dialkynyl-substituted 2,2'-bipyridine ligands: synthesis and structure of [{6,6'-(CH3CH2CH2C.tplbond.C)2bpy}Cu(Cl)(.mu.-Cl)]2

AU Koevari, Endre; Kraemer, Roland

CS Anorganisch-Chem. Inst., Univ. Muenster, Muenster, D-48149, Germany

SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1994), 49(10), 1324-8

CODEN: ZNBSEN; ISSN: 0932-0776

PB Verlag der Zeitschrift fuer Naturforschung

DT Journal

LA German

AB The bipyridyldiacetylene 6,6'-(CH3CH2CH2C.tplbond.C)2bpy (1) was prepd. by Pd catalyzed C-C-coupling reaction of 6,6'-dibromo-2,2'-bipyridine with pentyne. Reaction of 1 with anhyd. CuCl2 in MeCN gave the dimeric, chloro-bridged complex (1)Cu(Cl)(.mu.-Cl)2Cu(Cl)(1) (2), which was characterized by x-ray crystallog. The Cu atoms in 2 are square-pyramidally coordinated with normal in-plane Cu-N and Cu-Cl bond distances and one longer, apical bond to the 2nd bipyridyl N atom. The influence of steric hindrance of the bipyridyl 6,6'-substituents on the structure of the complex is discussed.

IT 159644-78-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and complexation with copper)

RN 159644-78-7 CAPLUS

CN 2,2'-Bipyridine, 6,6'-di-1-pentynyl- (9CI) (CA INDEX NAME)

$$n-\Pr-C = C \qquad N \qquad N \qquad C = C-\Pr-n$$

L6 ANSWER 36 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1995:182149 CAPLUS

DN 122:22538

TI Zinc(II) complexes of the ammonium-functionalized 2,2'-bipyridine [6,6-{Me2N(H)CH2C.tplbond.C}2bpy](ClO4)2 and of the related ligand 6,6'-(CH3CH2CH2C.tplbond.C)2bpy

AU Koevari, Endre; Kraemer, Roland

CS Anorg.-Chem. Inst., Univ. Muenster, Muenster, D-48149, Germany

SO Chemische Berichte (1994), 127(11), 2151-7 CODEN: CHBEAM; ISSN: 0009-2940

PB VCH

DT Journal

LA German

The 2,2-bipyridine deriv. 6,6'-(Me2NCH2C.tplbond.C)2bpy (1b) was prepd. by Pd-catalyzed C-C coupling reaction. Protonation of 1b with HX yielded [6,6'-{Me2N(H)CH2C.tplbond.C}2bpy]X2 (2a, X = NO3-; 2b, X = ClO4-). 2A was characterized by x-ray crystallog. (1A)ZnCl2 (3) and [(H21b)ZnCl2](ClO4)2 (4) were obtained by reaction of 2b and the related ligand 6,6'-(CH3CH2CH2C.tplbond.C)2bpy (1a) with ZnCl2. The crystal structure of 3 revealed a tetrahedral coordination of the metal ion by two bipyridine nitrogens and two chloride ligands. Stability consts. in MeCN/H2O (19:1) of the 1:1 Zn complexes of 1a and 2a were detd. spectrophotometrically. Complexes of [H21b]2+ are of potential interest as model systems for metal-NH4+ cooperatively in the active site of phosphodiesterase enzymes. In MeCN/H2O (19:1) the 1:1-species [(H21b)Zn] promotes the hydrolysis of bis(p-nitrophenyl) phosphate more efficiently than [(1a)Zn].

IT 159644-78-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (complexation with zinc)

RN 159644-78-7 CAPLUS

CN 2,2'-Bipyridine, 6,6'-di-1-pentynyl- (9CI) (CA INDEX NAME)

$$n-\Pr-C = C \qquad N \qquad N \qquad C = C-\Pr-n$$

IT 159644-79-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and complexation with zinc and protonation of)

RN 159644-79-8 CAPLUS

CN 2-Propyn-1-amine, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N-dimethyl- (9CI) (CA INDEX NAME)

$$Me_2N-CH_2-C = C$$
 N
 N
 $C = C-CH_2-NMe_2$

IT 159644-80-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and crystal structure of)

RN 159644-80-1 CAPLUS

CN 2-Propyn-1-amine, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N-dimethyl-, dinitrate (9CI) (CA INDEX NAME)

CM 1

CRN 159644-79-8 CMF C20 H22 N4

$$Me_2N-CH_2-C \equiv C$$
 N
 N
 $C \equiv C-CH_2-NMe_2$

CM 2

CRN 7697-37-2 CMF H N O3

IT 159644-81-2P

RN 159644-81-2 CAPLUS

CN 2-Propyn-1-amine, 3,3'-[2,2'-bipyridine]-6,6'-diylbis[N,N-dimethyl-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 159644-79-8 CMF C20 H22 N4

$$\texttt{Me}_2 \texttt{N} - \texttt{CH}_2 - \texttt{C} = \texttt{C} - \texttt{N} \\ \texttt{N} \\ \texttt{C} = \texttt{C} - \texttt{CH}_2 - \texttt{N} \\ \texttt{Me}_2 \\ \texttt{N} \\ \texttt{N} \\ \texttt{C} = \texttt{C} + \texttt{C} \\ \texttt{N} \\ \texttt{N}$$

CM 2

CRN 7601-90-3 CMF Cl H O4



L6 ANSWER 37 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1994:77782 CAPLUS

DN 120:77782

TI The palladium-catalyzed cross-coupling polymerization of diethynylmethyl (n-octyl)silane with dihaloarenes

AU Corriu, R. J. P.; Douglas, W. E.; Yang, Z. X.

CS Unite Mixte, CNRS, Montpellier, 34095, Fr.

SO European Polymer Journal (1993), 29(12), 1563-9 CODEN: EUPJAG; ISSN: 0014-3057

DT Journal

LA English

AB Polymers of structure -[-CCSi(MeOctn)CC-Z-]-n(Z = 1,4-benzene,4,4'-biphenyl, 9,10-anthracene, 2,7-fluorene, 2,5 and 2,6-pyridine, 6,6'-bipyridine, 2,5-thiophene, 2,6-p-dimethylaminonitrobenzene, 2,6-p-nitroaniline, 2,7-fluoren-9-one, p-tetrafluorobenzene, 2,6-p-nitrophenol or 2,6-p-cyanophenol) were prepd. by reaction of diethynylmethyl (n-octyl) silane with the appropriate hetero (arom.) dibromide or diiodide in the presence of (PPh3)2PdCl2 and CuI. The polymer where Z = 6,6'-bipyridine reacted with copper(II) trifluoromethanesulfonate to give a copper(II)-contg. polymer, redn. of which with hydrazine afforded the Cu(I)-contg. polymer. The effect of change in reaction conditions on the cross-coupling polymn. was investigated. High mol. wts. are favored by use of: (a) the diiodorather than the dibromoarene, (b) an equimolar mixt. of the reactants or excess diethynylsilane, and in most cases (c) toluene cosolvent. The mol. wt. passes through a max. as the total catalyst concn. is increased, or as the individual Cu and Pd catalyst concns. are sep. raised. The presence of tetraethylammonium chloride or high concns. of triphenylphosphine reduces the mol. wt.

RN 152194-87-1 CAPLUS

CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(methyloctylsilylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

RN 152194-87-1 CAPLUS

CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(methyloctylsilylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{Me-} (CH_2)7 \\
 & \text{C} & \text{C-} \text{Si-} \text{C} & \text{C} \\
 & \text{Me}
\end{array}$$

- L6 ANSWER 38 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1993:581384 CAPLUS
- DN 119:181384
- TI Preparation of oligomers containing tetraphenylsilole, acetylene and aromatic groups in the main chain, and incorporation of iron carbonyl
- AU Corriu, Robert J.-P.; Douglas, William E.; Yang, Zhi-xin
- CS Unite Mixte CNRS/Rhone Poulenc/UM II, CNRS UMR 44, Universite de Montpellier II Sciences et Techniques du Languedoc, Place Eugene Bataillon, Montpellier, 34095/5, Fr.
- SO Journal of Organometallic Chemistry (1993), 456(1), 35-9 CODEN: JORCAI; ISSN: 0022-328X
- DT Journal
- LA English
- Polycarbosilanes with the structure [-SiR2-C.tplbond.C-Z-C.tplbond.C]-n (R2Si = 2,3,4,5-tetraphenyl-1-sila-2,4-cyclopentadiene; Z = 1,4-benzene, 4,4'-biphenyl, 9,10-anthracene, 2,7-fluorene, 2,5- and 2,6-pyridine, 6,6'-bipyridine, 2,5-thiophene, 2,6-p-dimethylaminonitrobenzene, 2,6-p-nitroaniline, 2,6-p-nitrophenol, and 2,7-fluoren-9-one) were prepd. by reaction of 1,1-diethynyl-2,3,4,5-tetraphenyl-1-sila-2,4-cyclopentadiene with the appropriate (hetero)arom. dibromide or diiodide in the presence of [(PPh3)2PdCl2] and CuI. Exo- and endotherms obsd. in the initial DSC scans were absent in repeat scans. The oligomer where Z = p-C6H4 reacted with [Fe(CO)5] under UV irradn. to give an oligomer contg. iron carbonyl fragments attached to .apprx.30% of the silole groups.
- IT 150378-94-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (oligomers, prepn. and characterization of)

- RN 150378-94-2 CAPLUS
- CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(2,3,4,5-tetraphenylsilacyclopenta-2,4-dien-1-ylidene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

- L6 ANSWER 39 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1993:581376 CAPLUS
- DN 119:181376
- TI Preparation of diphenylsilylene polymers containing main-chain acetylene and (hetero)aromatic groups: .chi.(2) nonlinear optical and other properties
- AU Corriu, Robert J. P.; Douglas, William E.; Yang, Zhi-xin; Karakus, Yusuf; Cross, Graham H.; Bloor, David
- CS Unite Mixte CNRS/Rhone Poulenc/USTL, CNRS UMR 44, Universite de Montpellier II Sciences et Techniques du Languedoc, Place Eugene Bataillon, Montpellier, 34095/5, Fr.
- SO Journal of Organometallic Chemistry (1993), 455(1-2), 69-76 CODEN: JORCAI; ISSN: 0022-328X
- DT Journal
- LA English
- The title polymers, (C.tplbond.CSiPh2C.tplbond.CZ)n (I; Z = p-C6H4, AB 4,4'-biphenylyl, 9,10-anthracenediyl, fluorenediyl, 2,2'-bipyridine-6,6'diyl, pyridinediyl, 2,5-thiophenediyl, aminonitro-m-phenylene, hydroxynitro-m-phenylene, cyanohydroxy-m-phenylene, or p-C6F4) are prepd. by reaction of SiPh2(C.tplbond.CH)2 with the appropriate arylene dihalide in the presence of (PPh3)2PdCl2, CuI and PPh3, the solvent being either NEt3 or NEt3/PhMe. The av. mol. wts. of the polymers were 2600-34,000. The UV spectra have absorption max. at 250-400 nm. The I (Z = 2-(dimethylamino)-5-nitro-m-phenylene) is .chi.(2) active, r33 is 0.8 pm/V following fixed electrode poling at 17.5 V/.mu.m. The polymers do not melt below the decompn. temp., and all transitions shown in the DSC thermogram at .1toreq.300.degree. were absent on repeat scans. thermal dynamic anal. of I (Z = p-C6H4) indicated decompn. commencing at 290.degree. and continuing to .apprx.750.degree.. The residue was composed of .alpha.-SiC and amorphous C.
- IT 131151-44-5D, copper complexes
 - RL: PRP (Properties)

(characterization of)

- RN 131151-44-5 CAPLUS
- CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(diphenylsilylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

$$\begin{bmatrix} Ph \\ C = C - Si - C = C \\ Ph \end{bmatrix}$$

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and characterization of

10/087,066

L6 ANSWER 40 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1993:439449 CAPLUS

DN 119:39449

TI Synthesis, characterization and properties of novel covalently linked binuclear ruthenium(II) and trinuclear ruthenium(II)-copper(I) bipyridyl complexes

AU Grosshenny, Vincent; Ziessel, Raymond

CS Inst. Phys. Chim. Mater., Ec. Eur. Hautes Etud. Ind. Chim. Strasbourg, Strasbourg, 67008, Fr.

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1993), (5), 817-19 CODEN: JCDTBI; ISSN: 0300-9246

DT Journal

LA English

AB New ditopic ligands bearing 2 bipyridine subunits and an ethynyl or diethynyl bridge were synthesized and shown to form cationic mononuclear Ru(II) and Cu(I), dinuclear Ru(II), and trinuclear Ru(II)-Cu(I) complexes. The fluorescence of the complexes was studied.

IT 148353-62-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and fluorescence of)

RN 148353-62-2 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-N,N')[6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl-2,2'-bipyridine]-N,N']-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 148353-61-1 CMF C46 H38 N8 Ru CCI CCS

CM 2

CRN 16919-18-9

CMF F6 P CCI CCS

IT 133810-37-4P, 6-Ethynyl-5,5'-dimethyl-2,2'-bipyridine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with bromo analog)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)

IT 146548-28-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with ruthenium bipyridine complex)

RN 146548-28-9 CAPLUS

CN 2,2'-Bipyridine, 6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl- (9CI) (CA INDEX NAME)

IT 133810-36-3P, 6-Trimethylsilylethynyl-5,5'-dimethyl-2,2'-

bipyridine

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and removal of silyl group from)

RN 133810-36-3 CAPLUS

CN 2,2'-Bipyridine, 5,5'-dimethyl-6-[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 42 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1993:169307 CAPLUS

DN 118:169307

TI Synthesis and properties of novel ditopic polypyridine ligands bridged by one and two acetylenic bonds

AU Grosshenny, Vincent; Ziessel, Raymond

CS Inst. Phys. Chim. Mater., Ec. Eur. Hautes Ind. Chim., Strasbourg, 67008, Fr.

SO Tetrahedron Letters (1992), 33(52), 8075-8 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 118:169307

AB Ethynyl substituted bipyridine chelates react with bromo or triflate functionalized bipyridine or terpyridine subunits, in the presence of catalytic amts. of PdO(PPh3)4 to yield, the new homo- and heteroditopic ethynyl bridge ligands such as I (n = 1). Self coupling of the ethynyl substituted bipyridine species in the presence of CuCl/TMEDA/O2, yield the sym. diethynyl bridge ligands, such as I (n = 2). A ruthenium complex of I (n = 1) was reported. The application of such complexes in mol. electronic devices and photoinduced charge sepn. was mentioned (no data).

IT 133810-36-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and desilylation of)

RN 133810-36-3 CAPLUS

CN 2,2'-Bipyridine, 5,5'-dimethyl-6-[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

IT 133810-37-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and palladium-catalyzed coupling reaction of)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)

IT 146548-28-9P 146548-29-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 146548-28-9 CAPLUS

CN 2,2'-Bipyridine, 6,6''-(1,2-ethynediyl)bis[5,5'-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & C & C & N & N \\ \hline Me & Me & Me & Me \end{array}$$

RN 146548-29-0 CAPLUS

CN 2,2'-Bipyridine, 6,6''-(1,3-butadiyne-1,4-diyl)bis[5,5'-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & C = C - C = C \\ \hline Me & Me \\ \end{array}$$

10/087,066

- L6 ANSWER 44 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1992:49387 CAPLUS
- DN 116:49387
- TI Electrical conductivity of iron trichloride-doped poly(alkynylsilane)s
- AU Corriu, Robert J. P.; Douglas, William E.; Yang, Zhi Xin; Garnier, Francis; Yassar, Abderahim
- CS Univ. Montpellier II, Montpellier, 34095, Fr.
- SO Journal of Organometallic Chemistry (1991), 417(3), C50-C52 CODEN: JORCAI; ISSN: 0022-328X
- DT Journal
- LA English
- AB The elec. conductivities of [C.tplbond.CSiR1R2C.DELTA.C-Z]n (R1R!2Si = Ph2Si, nOct(Me)Si, 2,3,4,5-tetraphenyl-1-sila-2,4-cyclopentene; Z = (hetero)arom. group) doped with FeCl3 lie in the range 10-9 < .sigma. < 10-3 S cm-1, whereas those of the undoped polymers are less than 10-10 S cm-1. The presence of Ph groups on Si leads to increased cond.
- IT 131151-44-5

RL: PRP (Properties) (elec. cond. of)

- RN 131151-44-5 CAPLUS
- CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(diphenylsilylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

$$C = C - Si - C = C$$

$$Ph$$

$$Ph$$

$$Ph$$

10/087,066

L6 ANSWER 47 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1991:228682 CAPLUS

DN 114:228682

TI Towards molecular electronics: a new family of aromatic polyimine chelates substituted with alkyne groups

AU Suffert, Jean; Ziessel, Raymond

CS Lab. Stereochim. Organometall., EHICS, Strasbourg, 67000, Fr.

SO Tetrahedron Letters (1991), 32(6), 757-60 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

AB Pyridine derivs., e.g. (trimethylsilylethynyl)phenanthroline I, -dimethylbipyridine II and -naphthyridine III, were prepd. by reacting the bromo or chloropyridine deriv. with Me3SiC.tplbond.CH (IV) in the presence of Pd(PPh3)2Cl2/CuI. Thus, 5-bromo-1,10-phenanthroline reacts with IV to give I. The silylated products were deprotected to give the terminal acetylenes.

RN 133810-36-3 CAPLUS

CN 2,2'-Bipyridine, 5,5'-dimethyl-6-[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

RN 133810-37-4 CAPLUS

CN 2,2'-Bipyridine, 6-ethynyl-5,5'-dimethyl- (9CI) (CA INDEX NAME)

RN 133810-42-1 CAPLUS

CN 2,2'-Bipyridine, 6,6'-diethynyl- (9CI) (CA INDEX NAME)

RN 133810-47-6 CAPLUS

CN 2,2':6',2''-Terpyridine, 4'-phenyl-6,6''-bis[(trimethylsilyl)ethynyl]-(9CI) (CA INDEX NAME)

RN 133810-48-7 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-diethynyl-4'-phenyl- (9CI) (CA INDEX NAME)

RN 133826-69-4 CAPLUS

CN 2,2'-Bipyridine, 6,6'-bis[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)

- L6 ANSWER 48 OF 50 CAPLUS COPYRIGHT 2002 ACS
- AN 1991:24704 CAPLUS
- DN 114:24704
- TI Synthesis of poly(alkynylsilanes) having various aromatic groups in the backbone
- AU Corriu, Robert J. P.; Douglas, William E.; Yang, Zhi Xin
- CS Univ. Montpellier II Sci. Tech. Languedoc, Montpellier, 34095, Fr.
- SO Journal of Polymer Science, Part C: Polymer Letters (1990), 28(13), 431-7 CODEN: JSCLE2; ISSN: 0887-6258
- DT Journal
- LA English
- AB Polymers having the structure (-C.tplbond.CSi(Ph)2C.tplbond.CZ-)n (I; Z = p-C6H4, p-C6H4C6H4-p, 9,10-anthracenyl, 2,7-fluorenyl, 6,6'-bipyridinyl, 2,5- and 2,6-pyridinyl, and 2,5-thiophenyl) were prepd. by condensation of Ph2Si(C.tplbond.CH)2 with arom. dihalides in Et3N in the presence of (PPh3)2PdCl2, Cu2I2, and PPh3. Polymn. was complete after .apprx.16 h, which was confirmed by IR spectra. I was pptd. in pentane and characterized. No 1,3-butadiyne 13C NMR resonances were obsd., and no significant changes were obsd. after heating Ph2Si(C.tplbond.CH)2 under std. reaction conditions but in the absence of arom. dihalides.
- IT 131151-44-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and characterization of)

- RN 131151-44-5 CAPLUS
- CN Poly[[2,2'-bipyridine]-6,6'-diyl-1,2-ethynediyl(diphenylsilylene)-1,2- ethynediyl] (9CI) (CA INDEX NAME)

L6 ANSWER 49 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1990:178674 CAPLUS

DN 112:178674

TI Preparation of pyridyldialkanoic acids as leukotriene antagonist drugs

IN Young, Robert N.; Zamboni, Robert; Gauthier, Jacques Y.

PA Merck Frosst Canada, Inc., Can.

SO Eur. Pat. Appl., 29 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN. CNT 1

T. VIIA .	CIVI	1											
	PATENT NO.			KIND	DATE			APPLICATION NO.			DATE		
ΡI	EΡ	31808	3		A2	19890)531		ΕP	1988-20	2564	198811	116
	ΕP	31808	3		A3	19901	1205						
		R:	CH,	DE,	FR, GB	, IT,	LI,	NL					
	CA	13220	04		A1	19930	907		CA	1987-55	2754	198711	L25
	JP	01168	668		A2	19890	704		JP	1988-29	6381	198811	125
PRAI	CA	1987-	5521	754		19871	1125						

OS MARPAT 112:178674

The title compds. I [R1 = H, halo, alkyl, alkenyl, alkynyl, CF3, SOR2, SO2R2, SR2, NR32, OR3, CO2R3, etc.; R2 = alkyl, alkenyl, alkynyl, CF3, (un) substituted Ph, etc.; R3 = H, R2; R4 = H, halo, NO2, CN, etc.; CR3R4 = amino acid radical; R5 = H, halo, CN, SR2, OR3, etc.; R6 = (CH2)sCR72 (CH2)s R8, CH2CONR92; R7 = H, alkyl; R8 = heterocyclyl; X1, X2 = O, S, SO, SO2, etc.; Y = CR2:CR3, C.tplbond.C, etc.; Z1, Z2 = CONR3, phenylene, etc.; Q1, Q2 = CO2R3, CHO, tetrazolyl, etc.; m, p = 0, 1-8; n, r = 0, 1; s = 0, 1-3] are prepd. as leukotriene formation-inhibiting drugs, useful as anti-inflammatory antiasthmatic and antiallergic agents (no data). 3-[2-(5-Phenylpyridin-2-yl)ethenyl]benzaldehyde (prepn. given) was reacted with (prepn. given) was reacted with Me 3-mercaptopropionate, in BF3.Et2O-contg. CH2Cl2, at 0.degree., to give di-Me 5-[3-[2-(5-phenylpyridin-2-yl)ethenyl]phenyl]-4,6-dithianonanedioate. This was sapond. with LiOH and converted into the di-Na salt.

IT 126268-51-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as leukotriene formation-inhibiting drug)

RN 126268-51-7 CAPLUS

CN Benzoic acid, 3-[[(2-carboxyethyl)thio][3-[(5-chloro-6-phenyl-2-pyridinyl)ethynyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$C1$$
 $CH_2-CH_2-CO_2H$
 CH_2
 CO_2H

L6 ANSWER 50 OF 50 CAPLUS COPYRIGHT 2002 ACS

AN 1989:115570 CAPLUS

DN 110:115570

TI Preparation and thermal polymerization of oligomeric poly(oxypyridinediyloxyarylenes bearing terminal acetylene groups

IN Dussart-Lermusiaux, Annie; Senneron, Michel; Rabilloud, Guy; Sillion, Bernard

PA Centre d'Etude des Materiaux Organiques pour Technologies Avancees, Fr.

SO Fr. Demande, 26 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE					
PI	FR 2605010	A1	19880415	FR 1986-14090	19861009					
	FR 2605010	· B1	19881230	••						
	FR 2621041	A2	19890331	FR 1987-13405	19870925					
	FR 2621041	B2	19900112							
	EP 267076	A1	19880511	EP 1987-402209	19871006					
	R: BE, CH,	DE, GB	, IT, LI, NL							
	US 4814403	A	19890321	US 1987-105745	19871008					
	JP 63117034	A2	19880521	JP 1987-256139	19871009					
PRAI	FR 1986-14090		19861009							

The title oligomers, useful in composites, adhesives, foams, etc., are prepd. by polymg. bisphenol salts with dihalopyridines and ethynylation of the halogen-terminated products. Heating 0.4 mol 2,6-dibromopyridine with 0.2 mol resorcinol and 41.49 g K2CO3 in N-methylpyrrolidone-PhMe at 130.degree. for 7 h with azeotropic distn. of H2O gave 91% 6,6'-(m-phenylenedioxy)bis(2-bromopyridine), catalytic condensation of which with 2-methyl-3-butyn-1-ol gave 66% bis(3-hydroxy-3-methyl-1-butynyl) deriv., alk. degrdn. of which gave 50% 2,2'-(m-phenylenedioxy)bis(6-ethynylpyridine) (I). Heating I at 180.degree. for 2 h gave a polymer with initial decompn. temp. (TGA) 356 and 379.degree. in air and Ar, resp., and wt. loss after 20 h at 300.degree. 2.7%.

IT 119421-85-1P 119421-86-2P 119421-88-4P

119421-89-5P

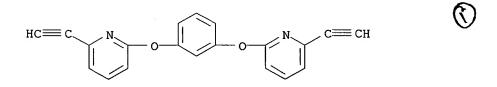
RL: IMF (Industrial manufacture); PREP (Preparation)
 (heat-resistant, manuf. of)

RN 119421-85-1 CAPLUS

CN Pyridine, 2,2'-[1,3-phenylenebis(oxy)]bis[6-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 119409-37-9 CMF C20 H12 N2 O2



RN 119421-86-2 CAPLUS

CN Pyridine, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[6-ethynyl-,

homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 119409-38-0 CMF C29 H22 N2 O2 Gropino (A)

RN 119421-88-4 CAPLUS

CN Pyridine, 2,2'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[6-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 119421-98-6 CMF C29 H16 F6 N2 O2 Q polices S

RN 119421-89-5 CAPLUS

CN Pyridine, 2,2'-[thiobis(4,1-phenyleneoxy)]bis[6-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 119409-40-4 CMF C26 H16 N2 O2 S Oarivar P

IT 119409-36-8P 119409-39-1P

RL: IMF (Industrial manufacture); PREP (Preparation) (manuf. and degrdn. of)

RN 119409-36-8 CAPLUS

CN 3-Butyn-2-ol, 4,4'-[1,3-phenylenebis(oxy-6,2-pyridinediyl)]bis[2-methyl-(9CI) (CA INDEX NAME)

RN 119409-39-1 CAPLUS

IT 119409-37-9P 119409-38-0P

RL: IMF (Industrial manufacture); PREP (Preparation)
 (manuf. of)

RN 119409-37-9 CAPLUS

CN Pyridine, 2727 [1,3-phenylenebis (oxy)]bls[6-ethynyl- (9CI) (CA INDEX NAME)

RN 119409-38-0 CAPLUS

CN Pyridine, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[6-ethynyl-(9CI) (CA INDEX NAME)

IT 119409-40-4P 119421-98-6P

RL: PREP (Preparation) (prepn. of)

RN 119409-40-4 CAPLUS

CN Pyridine, 2,2'-[thiobis(4,1-phenyleneoxy)]bis[6-ethynyl- (9CI) (CA INDEX NAME)

RN 119421-98-6 CAPLUS

CN Pyridine, 2,2'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[6-ethynyl- (9CI) (CA INDEX NAME)

$$HC \equiv C$$
 CE_3
 CE_3
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